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SOME ANALYTICAL SOLUTIONS FOR RAYLEIGH WAVES IN CUBIC CRYSTALS†

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As analytical solution of the problem of the propagation of Rayleigh waves in cubic crystals in their elastic symmetry planes and in the directions of the crystallographic axes is constructed using a three-dimensional complex formalism. The Rayleigh function is analysed taking into account the multiplicity of the roots of the characteristic polynomials, and the conditions under which it approaches zero for two values of the phase velocity are investigated. The relations between the elasticity constants of the cubic crystals for which a Rayleigh wave cannot propagate in the direction of the crystallographic axes are obtained.

The propagation of Rayleigh waves on the surface of anisotropic crystals was investigated for the first time by Stoneley [1] using Rayleigh's method [2]. The case of surface waves propagating in the elastic symmetry planes in the direction of the crystallographic axes of cubic crystals and along the diagonals to them was considered. When determining the roots of the characteristic polynomials, it was assumed, as in the isotropic case [2], that they are pure imaginary. It was shown [3–5] that the roots of the polynomials for cubic crystals, generally speaking, are complex. Later, Rayleigh's analytical methods were extended to hexagonal crystals [6] and orthohombic crystals [7].

Other versions of the analytical approach to investigating Rayleigh waves in the elastic symmetry planes and highly symmetric directions of cubic crystals and also close to these directions are known [8–11]. An asymptotic method has been developed which reduces the Rayleigh-wave problem in a medium with weak anisotropy to a Rayleigh-wave problem in an elastic isotropic half-space [12–13].

Of the various numerical solutions we note investigations on determining the velocities of Rayleigh waves propagating in different planes of cubic and hexagonal crystals [14–16].

The physical properties and characteristics of the different types of surface acoustic waves have been systematically described in [17], where they are also classified. Note that beginning with Stoneley's paper [1], in all subsequent publications [3–17] the case when there are multiple roots, corresponding to one-dimensional spectral spaces, among the roots of the characteristic polynomial were not considered. This has a led to a loss of one important class of solutions.

In this paper we use a classical approach, which goes back to Rayleigh, in which any possible change in the structure of the solution corresponding to multiple roots, is ignored.

1. FUNDAMENTAL EQUATIONS

The equations of motion for an anisotropic medium have the form

$$\operatorname{div}\mathbf{C}\cdot\cdot\nabla\mathbf{u} = \rho\ddot{\mathbf{u}} \tag{1.1}$$

where C is the four-valent elasticity tensor, ρ is the density of the medium, and $\mathbf{u}$ is the displacement field. The solution for the partial components of the Rayleigh wave can be expanded in the form

$$\mathbf{u}(\mathbf{x}) = \mathbf{m}e^{i\gamma\mathbf{v}\cdot\mathbf{x}}e^{i(\varkappa\mathbf{n}\cdot\mathbf{x}-\omega t)} \tag{1.2}$$

where $\mathbf{m}$ is the amplitude vector, γ is the (complex) root of the characteristic polynomial of Christofel's equation, ν is the vector of the unit outward normal to the plane in which the surface wave propagates, $\mathbf{n}$ is the unit vector which defines the direction of propagation of the wave, $\varkappa$ is the wave number and ω is the frequency of the wave.

Substituting (1.2) into (1.1) we obtain

$$\mathbf{T}\cdot\mathbf{m} = 0 \tag{1.3}$$

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where

$$\mathbf{T} = \gamma^2\mathbf{A} + \gamma\mathbf{B} + \mathbf{D}$$
$$\mathbf{A} = \boldsymbol{\nu}\cdot\mathbf{C}\cdot\boldsymbol{\nu},\ \ \mathbf{B} = \boldsymbol{\nu}\cdot\mathbf{C}\cdot\mathbf{n} + \mathbf{n}\cdot\mathbf{C}\cdot\boldsymbol{\nu},\ \ \mathbf{D} = \mathbf{n}\cdot\mathbf{C}\cdot\mathbf{n}-\mathbf{I}\rho c^2,\ c = \omega/\varkappa \tag{1.4}$$

and **I** is identity matrix.

In order for (1.3) to be satisfied when $\mathbf{m} \neq 0$, it is necessary and sufficient that

$$\det\mathbf{T} = 0 \tag{1.5}$$

Condition (1.5) reduces to a sixth-order polynomial equation in γ. Substituting the roots with negative imaginary part, which we will denote by ξ_k, into (1.3), we obtain the eigenvectors $\mathbf{m}^{(k)}$ corresponding to these roots. The displacement vector will be sought in the general case in the form of a linear combination of three eigenvectors (or three waves)

$$\mathbf{u} = \sum_{k=1}^{3} X_k\mathbf{m}^{(k)}F(\xi_k),\ \ F(\xi_k) = \exp(-i\xi_k\mathbf{x}\cdot\boldsymbol{\nu} + i\varkappa(\mathbf{x}\cdot\mathbf{n} - ct)) \tag{1.6}$$

where X_k are arbitrary (complex) coefficients.

Note. In this paper we investigate the case when Eq. (1.5) has three pairs of complex-conjugate roots, to which correspond three eigenvectors $\mathbf{m}_k$. Other cases have been considered previously.†

The boundary conditions corresponding to a stress-free surface

$$\boldsymbol{\nu}\cdot\mathbf{C}\cdot\cdot\nabla\mathbf{u} = 0 \tag{1.7}$$

must be satisfied on the surface of the medium.

Substituting (1.6) into (1.7) we obtain a matrix equation in the unknown coefficients X_k

$$\mathbf{H}\cdot\mathbf{X} = 0,\ \ \mathbf{X} = (X_1, X_2, X_3) \tag{1.8}$$

where **H** is a 3×3 complex-significant matrix. The necessary and sufficient condition for non-trivial solutions of Eq. (1.8) to exist is as follows:

$$\det\mathbf{H} = 0 \tag{1.9}$$

from which we can obtain the Rayleigh-wave velocity c_R.

It is assumed that the elasticity tensor **C** is *positive definite*

$$\forall\mathbf{A} \in \mathrm{sym}(R^3 \otimes R^3),\ \ \mathbf{A} \neq 0$$
$$(\mathbf{A}\cdot\cdot\mathbf{C}\cdot\cdot\mathbf{A}) \equiv \sum_{i,j,m,n} A_{ij}C^{ijmn}A_{mn} > 0 \tag{1.10}$$

In addition a supplementary *positive definite* condition is imposed on the elasticity tensor. In order to introduce this condition, consider the convolution

$$(\mathbf{C}**\mathbf{A})^{in} = \sum_{j,m} C^{ijmn}A_{jm} \tag{1.11}$$

where A is a symmetric positive definite second-rank tensor. In terms of convolution (1.11) the supplementary positive definite condition has the form

$$\forall\mathbf{A} \in \mathrm{sym}(R^3 \otimes R^3),\ \ \mathbf{A} \neq 0$$
$$(\mathbf{A}**\mathbf{C}**\mathbf{A}) \equiv \sum_{i,n,j,m} A_{in}C^{ijmn}A_{jm} > 0 \tag{1.12}$$

An analysis of conditions (1.10) and (1.12) shows that in the general case of anisotropy, one of these does not follow from the other.

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All actual anisotropic materials obviously satisfy condition (1.12). An analysis of different systems of crystals [18] does not reveal any breakdown of the supplementary positive definite condition.

2. STONELEY'S SOLUTION

For cubic crystals we have three independent moduli of elasticity

$$C_{1111} = C_{2222} = C_{3333} = C_{11}, \ C_{1122} = C_{1133} = C_{2233} = C_{12}$$
$$C_{1212} = C_{1313} = C_{2323} = C_{44}$$

Before continuing with the further analysis we will write the condition for the elasticity tensor $\mathbf{C}$ to be positive definite

$$C_{11} > 0, \ C_{44} > 0, \ -C_{11}/2 < C_{12} < C_{11} \tag{2.1}$$

The supplementary positive definite condition has the form

$$C_{11} - C_{44} > 0, \ C_{12} + C_{44} > 0, \ C_{11} + 2C_{44} > 0$$

Equation (1.5) for a cubic crystal corresponds to the two equations

$$C_{44} + C_{44}\gamma^2 - \rho c^2 = 0, \quad a\gamma^4 + b\gamma^2 + r = 0 \tag{2.2}$$

The parameters a, b and r are related to the elasticity constants and the phase velocity by the equations

$$a = C_{11}C_{44}, \ b = C_{11}^2 - C_{12}^2 - 2C_{12}C_{44} - (C_{11} + C_{44})\rho c^2$$
$$r = C_{12}C_{44} - (C_{11} + C_{44})\rho c^2 + \rho^2 c^4 \tag{2.3}$$

One pair of roots of the equation is found from the first equation of (2.2); in order that it should be complex, it is necessary and sufficient that

$$c < \sqrt{C_{44}/\rho} \equiv c_3 \tag{2.4}$$

where c_3 is the velocity of the slow transverse wave. The other roots are found from the second equation of (2.2).

Substituting the roots with negative imaginary parts (ξ_2 from the first equation of (2.2) and ξ_1 and ξ_3 from the second) into (1.3), we obtain the eigenvectors corresponding to these roots. Following the procedure described above (formulae (1.6)–(1.9)), the details of which can be found in Stoneley's paper [1] (see also [6]), we obtain the condition for the determinant of boundary conditions (2.10) to vanish reduces to the following

$$X_2 = 0 \tag{2.5}$$

$$\det \mathbf{H} = \frac{C_{44}(\xi_1 - \xi_3)}{(C_{11} + C_{44})^2 \xi_1 \xi_3} G(\xi_1, \xi_2) = 0, \ \alpha = C_{11} - \rho c^2$$

$$G(\xi_1, \xi_3) = \{-C_{12}C_{11}C_{44}\xi_1^2\xi_3^2 + \alpha C_{11}C_{44}(\xi_1^2 + \xi_3^2) - \tag{2.6}$$
$$- \xi_1, \xi_3(C_{12} + C_{44})(C_{12}^2 - \alpha C_{11}) - \alpha[C_{12}(C_{12} + C_{44}) - C_{11}\alpha]\}$$

It follows from (2.5) that there is no partial component in the surface wave corresponding to a wave polarized perpendicular to the sagittal plane (the plane formed by the vectors $\boldsymbol{\nu}$ and $\mathbf{n}$). If the roots ξ_1, ξ_3 are different (as was assumed in [1]), equating the determinant of the boundary conditions to zero corresponds to the equation

$$G(\xi_1, \xi_2) = 0 \tag{2.7}$$

Since for a biquadratic equation the two pairs of complex-conjugate roots differ from one another in sign, we have

$$\xi_1^2\xi_3^2 = r/a, \ \ \xi_1^2 + \xi_3^2 = -b/a \tag{2.8}$$

and from conditions (2.3), (2.7) and (2.8) we obtain the condition [1] from which we can find the Rayleigh-wave velocity c_R

$$R^2(1-R)=\left[1-\left(\frac{C_{12}}{C_{11}}\right)^2-R\right]^2\left(1-\frac{C_{11}}{C_{44}}R\right),\quad R=\frac{\rho c_R^2}{C_{11}} \tag{2.9}$$

We can obtain the expression (6)

$$x=\frac{X_3}{X_1}=-\frac{\xi_3(C_{12}\xi_1^2-C_{11}+\rho c_R^2)}{\xi_1(C_{12}\xi_3^2-C_{11}+\rho c_R^2)} \tag{2.10}$$

from which it follows that if $\xi_1 \to \xi_3$ then $x \to -1$. It can also be shown that when $\xi_1 \to \xi_3$ the components of the eigenvectors $\mathbf{m}^{(1)}$ and $\mathbf{m}^{(3)}$ approach one another (since they are represented by the same expressions, which depend on the roots ξ_1 and ξ_2, respectively).

The result obtained can be formulated in the form of the following proposition: if $\xi_1 \to \xi_3$, the ratio of the amplitudes of the two eigenvectors which comprise the Rayleigh wave approach -1 and $\mathbf{m}^{(1)} \to \mathbf{m}^{(3)}$.

Corollary. Under the conditions of this assumption $X_1\mathbf{m}^{(1)} + X_3\mathbf{m}^{(3)} \to 0$.

3. MULTIPLE ROOTS

We will now consider the case when the second of equations (2.2) has a multiple root. This is possible if its discriminant vanishes, which leads to the condition

$$b^2-4ar=0 \tag{3.1}$$

The case of a generalized Rayleigh wave corresponds to a negative value of discriminant (3.1), while the usual Rayleigh wave corresponds to the positive case [9].

Equation (3.1) can be written in the form of a biquadratic equation

$$\begin{gathered}\rho^2 a_1 c^4+\rho b_1 c^2+r=0\\ a_1=(C_{11}-C_{44})^2,\ b_1=2(C_{11}+C_{44})B,\ B=(C_{12}+2C_{44}-C_{11})(C_{11}+C_{12})\\ r_1=\left(C_{12}^2-C_{11}^2\right)\left[(C_{12}+2C_{44})^2-C_{11}^2\right]\end{gathered} \tag{3.2}$$

from which one can obtain the value of the velocity or which the roots become multiple. If the discriminant of Eq. (3.2) is positive and $r_1 < 0$, which is equivalent to the inequality

$$C_{44} > (C_{11}-C_{12})/2 \tag{3.3}$$

a positive root of Eq. (3.2) exists which is expressed by the formula

$$c_a=\frac{\left(-(C_{11}+C_{44})X+22\,|\,C_{12}+C_{44}\,|\sqrt{C_{11}C_{44}B}\right)^{1/2}}{\sqrt{\rho}\,|\,C_{11}-C_{44}\,|} \tag{3.4}$$

Hence, we can formulate the following propositions

1. if $c_a < c_3$, $c_R \neq c_a$ the determinant of the boundary conditions (2.6) vanishes when $c \to c_a$;

2. the wave corresponding to the phase velocity for which a multiple root occurs does not exist, since the partial waves we have $X_1\mathbf{m}^{(1)}F(\xi_1) + X_3\mathbf{m}^{(3)}F(\xi_3) \to 0$ as $c \to c_a$.

The latter follows from the corollary to the proposition derived at the end of Section 2.

4. RESULTS OF CALCULATIONS

The Rayleigh functions for some cubic crystals. We will consider crystalline aluminium as an example. We will take the following values as the moduli of elasticity: $C_{11} = 0.10730 \times 10^{12}$ N/m^2, $C_{12} = 0.609 \times 10^{11}$ N/m^2 and $\rho = 2.6996 \times 10^9$ kg/m^3.

In Fig. 1 we show a graph of the Rayleigh function (RF) (this is what we will call the modulus of the determinant of boundary conditions (2.6) below) as a function of the phase velocity. It can be seen that

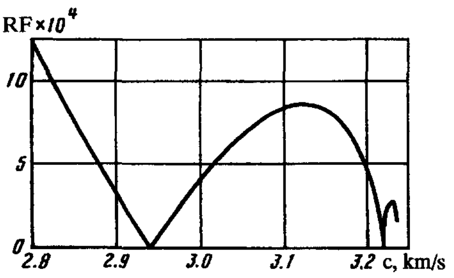

Fig. 1.

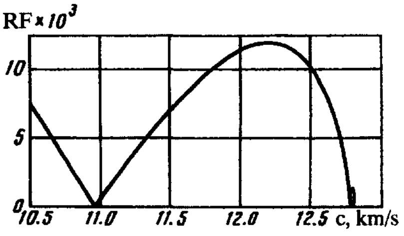

Fig. 2.

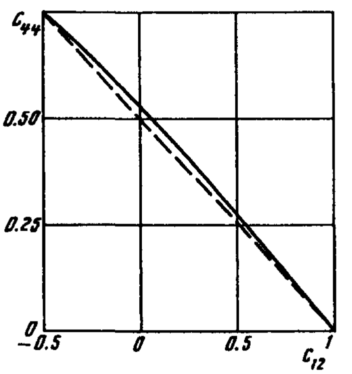

Fig. 3.

the Rayleigh function tends to zero for two values of the velocity: $c_R = 2941$ m/s (this is also the velocity of the surface wave) and $c_a = 3219$ m/s. The first value of the velocity agrees with the well-known result [14]. The second corresponds to the occurrence of multiple roots. Note that the velocity of the transverse wave for aluminium is 3238 m/s.

In Fig. 2 we show a graph of the Rayleigh function against the phase velocity c in the region of the limiting value, corresponding to the velocity of propagation of a transverse wave for a diamond crystal. We took the following characteristics of the material [14]: $C_{11} = 0.10760 \times 10^{13}\ \mathrm{N/m^2}$, $C_{12} = 0.12500 \times 10^{12}\ \mathrm{N/m^2}$, $C_{44} = 0.57535 \times 10^{12}\ \mathrm{N/m^2}$ and $\rho = 3.5095 \times 10^9\ \mathrm{kg/m^3}$. It can be seen that, in this case also, there are two values of c for which the Rayleigh function vanishes. These values are 10,973 m/s and 12,780 m/s. The velocity of the transverse wave is 12,804 m/s.

To compare the results with those obtained in [14] we also investigated a whole series of other crystals. However, this behaviour of the Rayleigh function was only found in the two materials mentioned. This is due to the fact that these materials are slightly anisotropic and the velocity for which the roots become multiple is less than the velocity of propagation of transverse waves in this direction. These results were not mentioned in [14], which is apparently due to the insufficient accuracy of the numerical algorithm employed.

The Rayleigh function of model materials. We will investigate the case when the velocity of a Rayleigh wave c_R is identical with the velocity c_a for which multiple roots are formed. To do this we substitute (3.4) into (2.9). The equation obtained is satisfied for certain relations between the other moduli C_{11}, C_{12} and C_{44}. This relation is shown in Fig. 3 by the continuous line in the form of a graph of C_{44} against C_{12} when $C_{11} = 1$. For comparison we show the values of C_{44} for which the elastic medium becomes isotropic (the dashed curve). It can be seen that the range of moduli of elasticity for which a Rayleigh wave is forbidden corresponds to slightly isotropic crystals.

The results obtained can be presented as follows: a Rayleigh surface wave cannot propagate when the vectors of its wave components become antiparallel; the necessary condition for this is that the velocity of the Rayleigh wave should be identical with the velocity for which the roots of the characteristic polynomial become multiple.

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